CHEMISTRY OF USE & PROCESS DESCRIPTION

OVERVIEW: The Chemistry of Use & Process Description module identifies the chemical, physical, and mechanical properties which contribute to the effectiveness of the use cluster chemicals or technologies in an industry- or product-specific application. The module also details the process in which the chemicals are used through the creation of a process flow diagram that schematically describes the process operations, equipment, and material flows.

GOALS:

- Identify the characteristics of a chemical (e.g., low vapor pressure, high solvency, water solubility, ductility, and other chemical, physical, or mechanical chemical properties) that contribute to its effectiveness in achieving the desired function.
- Develop a process flow diagram that describes each operation performed in the application being evaluated.
- Utilize the chemistry of use and process flow diagram to identify potential substitute chemicals, processes, or technologies.
- Provide a basis for developing a survey instrument to evaluate workplace practices in the use cluster industry and to determine the possible sources of chemical release in the use cluster.

PEOPLE SKILLS: The following lists the types of skills or knowledge that are needed to complete this module.

- Knowledge of basic chemical properties and reactions.
- Ability to create and use process flow diagrams.
- Knowledge of the manufacturing, commercial, or industrial process that is being evaluated.

Within a business or DfE project team, the people who might supply these skills include a chemist, process operator, process supervisor, or a chemical or mechanical engineer. Vendors of any process chemicals or equipment may also be a good resource.

DEFINITION OF TERMS:

<u>Flow Diagram</u>: A block diagram that depicts the equipment, material streams, and basic operations performed in a process.

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<u>Material Stream</u>: A flow of material (e.g., water, chemicals, product outputs, air emissions, etc.) either into or out of a step in the process.

<u>Unit Operation</u>: A process step that achieves a desired function.

APPROACH/ METHODOLOGY: The following presents a summary of the approach or methodology for evaluating the chemistry of use and preparing a process description. If there are substantially different methods of performing the use cluster function within an industry, it may be necessary to define the chemistry of use and prepare a process description for each of the methods typically employed. Further methodology details for Step 4 follow this section.

- Step 1: Obtain chemical data including CAS RNs, molecular structure, and chemical/physical properties from the Chemical Properties module.
- Step 2: Identify the properties that contribute to the effectiveness of the use cluster chemicals or technologies in performing the desired function. The properties may be chemical properties (e.g., a solvent with the ability to dissolve many different types of resins may be required in a paint stripping product), physical properties (e.g., a printing ink may have to be white, thus requiring the ink to contain a white pigment, such as titanium dioxide), or mechanical properties (e.g., a material substrate may need to meet specific mechanical qualifications for yield strength or fracture toughness). These properties are important criteria when selecting alternatives for a particular use cluster and identifying performance characteristics for the Performance Assessment.
- Step 3: Examine the industry- or product-specific application of the use cluster chemicals to identify the following:
 - Unit Operations, or process steps, required to perform the desired function (e.g., cleaning, degreasing, plating, product assembly, drilling, painting, drying, etc.). Identify any chemical, physical, or mechanical agents used in conjunction with the use cluster chemicals (e.g., dilution with water, heat, pressure, mechanical agitation, etc.).
 - Equipment used in the process steps (e.g., production machinery, reactors, heaters, waste stream control technologies, etc.).
 - Material streams that flow into, out of, or between steps in the process (e.g., raw material inputs, product outputs, rinse water streams, solid waste disposal, air emissions, waste water discharges, etc.).
 - The manner in which raw materials, chemicals, or products are stored and handled (e.g., chemical feedstock handling, methods of storage, etc.).
 - Any other data that might be necessary to prepare a process description or process flow diagram.
- Step 4: Construct a process flow diagram using the information collected in Step 3. An example flow diagram is shown in the Methodology Details section.

- Step 5: Review the information obtained from Steps 1 through 4 with the objective of identifying alternative chemicals, processes, and/or technologies (i.e., substitutes) that could be used to accomplish the same function. One approach to identifying substitutes is to consult with other industries that have similar functional requirements at some stage in the manufacturing or commercial service process. Another approach is to consult with vendors of chemicals or equipment who may be able to suggest process improvements that reduce environmental releases. Also, consult technical assistance organizations that have a broad overview of chemical uses and substitutes in many different industries.
- Step 6: Transfer a description of the unit operations and the process flow diagram to the following modules:
 - Workplace Practices & Source Release Assessment.
 - Process Safety Assessment.
 - Exposure Assessment.
 - Regulatory Status.
 - Pollution Prevention Opportunities Assessment.
 - Control Technologies Assessment.
 - Performance Assessment.
- Step 7: Provide data on material streams (e.g., water, raw materials, chemicals, etc.) to the Resource Conservation module, and a list of equipment used in the process to the Energy Impacts module.

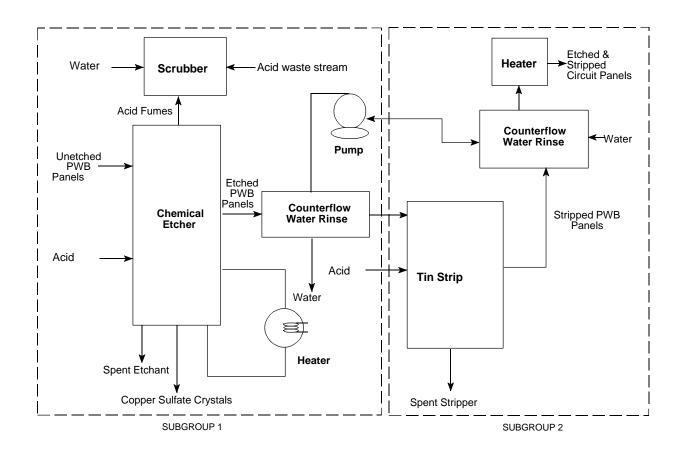
METHODOLOGY DETAILS: This section presents the methodology details for completing Step 4.

Details: Step 4, Process Flow Diagram Example

Figure 5-7 is an example of a process flow diagram for the pattern etching use cluster of the printed wiring board manufacturing process.

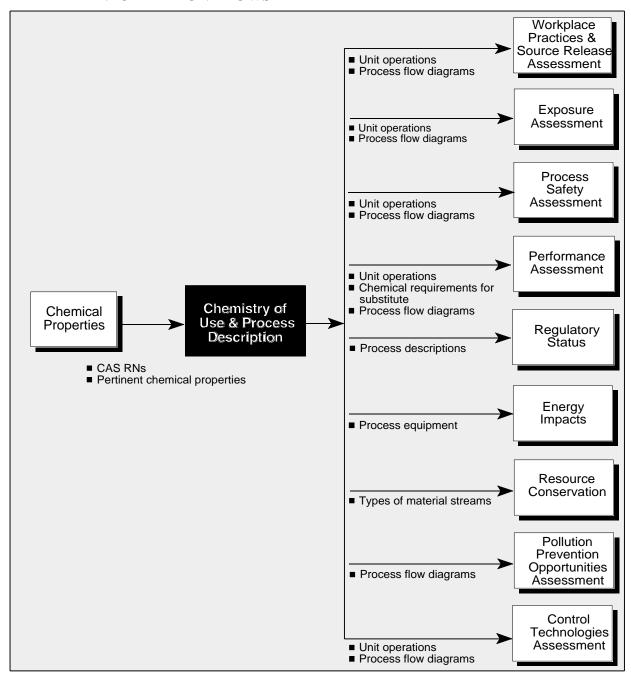
The pattern etching use cluster begins with the chemical etching of the unetched circuit panels and ends with the final drying of the etched panel. The use cluster shown here has the functional subgroups of chemical etching (Subgroup 1) and tin resist stripping (Subgroup 2). Subgroup 1 includes the actual etching step as well as a rinsing step to remove the excess etchant from the panels. Subgroup 2 includes the actual tin-resist stripping process step and a rinsing and drying step performed before the etched circuits can pass to the next step in the printed wiring board manufacturing process.

FIGURE 5-7: EXAMPLE PROCESS FLOW DIAGRAM OF A PATTERN ETCH PROCESS FOR PWB MANUFACTURING



FLOW OF INFORMATION: In a CTSA, this module receives information from the Chemical Properties module and transfers information to the Workplace Practices & Source Release Assessment, Exposure Assessment, Process Safety Assessment, Performance Assessment, Regulatory Status, Energy Impacts, Resource Conservation, Pollution Prevention Opportunities Assessment, and Control Technologies Assessment modules. Example information flows are shown in Figure 5-8.

FIGURE 5-8: CHEMISTRY OF USE & PROCESS DESCRIPTION MODULE: EXAMPLE INFORMATION FLOWS



ANALYTICAL MODELS: None cited.

PUBLISHED GUIDANCE: Although no publications were identified that provide guidance for this module, chemical engineering textbooks explain the basic concepts of process flow diagrams and provide numerous examples. Table 5-17 lists a few examples of chemical engineering textbooks.

TABLE 5-17: PUBLISHED GUIDANCE ON CHEMISTRY OF USE & PROCESS DESCRIPTION	
Reference	Type of Guidance
Himmelblau, David M. 1990. Basic Principles and Calculations in Chemical Engineering.	Examples of process flow diagrams.
Luyben, William and L. Wenzel. 1988. Chemical Process Analysis: Mass and Energy Balances.	Examples of process flow diagrams.

Note: References are listed in shortened format, with complete references given in the reference list following Chapter 10.

DATA SOURCES: None cited.